Trichloroethylene

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 6.44 days

Global applicability domain: Inside

Local applicability domain index: 6.59e-01

Confidence level: 6.90e-01

Nearest Neighbors from the Training Set

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Methylcyclopentane
Measured: 24.3
Predicted: 4.41

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Ethylcyclopentane
Measured: 511
Predicted: 8.14

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1,3-Dimethylcyclopentane
Measured: 24.3
Predicted: 4.08

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1,2-Dimethylcyclopentane
Measured: 24.3
Predicted: 4.46

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1,1-Dimethylcyclopentane
Measured: 880
Predicted: 10.9